# USER GUIDE

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# 1 *INT***RODU***CTI***ON***

## *1.1 Background*

Large volumes of freshly broken and crushed sulphide-bearing rock are discarded as waste at metalliferous mine sites. This material commonly gives rise to contamination of surface and groundwater by high concentrations of trace metals and other potentially harmful elements. MINDEC provides a decision-support tool for environmental planners and regulators concerned with the management of mine wastes and with the contamination of waters arising from those wastes. MINDEC has been developed with funding from the UK Department for International Development (DFID) under the KAR (Knowledge and Research) programme, project R7118: 'Cost Effective Evaluation of Hazards from Mine Waste'. It has been developed primarily for use in situations where the resources available for on-site data collection may be insufficient for a full assessment of a large number of sites.

The program can be used:

- to prioritise mine waste sites for further study/monitoring and/or remediation work on the basis of the threat that these sites pose to ground and surface water quality and to the health of water consumers;
- to provide guidance concerning the relative risks associated with using different water sources at a receptor site;
- to predict whether groundwater at the receptor site is likely to deteriorate in quality in the future;
- to aid in the development of more complete conceptual models of contaminant migration at individual sites;
- as a predictive tool to provide some indication of water quality at a hypothetical receptor site (such as a planned water supply borehole that has not yet been constructed); or,
- to carry out human health risk assessments of the water pathway using actual contaminant concentrations at a receptor site (where these data are available).

MINDEC considers mine waste contaminant migration in terms of:

- a source; i.e. the mine waste;
- a pathway; i.e. a surface waterway or a groundwater body;
- a receptor; which might be, for example, a surface water body, a water well or a water consumer.

MINDEC provides a 'best estimate' of the threat to ground and surface water quality and to the health of water consumers at a distant receptor site by calculating:

- expected concentrations at the receptor site of a suite of potentially harmful trace elements in waters originating from the mine waste site under study;
- human health risk indices (toxic hazard quotients and for arsenic a carcinogenic risk factor) for consumers of the contaminated waters;
- a water quality standard (WQS) exceedance index, which provides an indication of the extent to which the expected concentrations at the receptor exceed water quality standards;
- relative contaminant-element doses (as percentages of the total dose) from surface water, groundwater and other water sources.

The program also gives some indication of:

- contaminant travel times from the mine waste source to the receptor through the groundwater pathway;
- the expected duration of contaminant generation at the mine waste site.

## *1.2 Limitations*

In order to accommodate the wide variety of conditions at different mine sites MINDEC takes a necessarily simplistic approach to site assessment. It should be emphasised that, due to the assumptions involved in the calculations (see ***2.3 Assumptions***) **the results presented by MINDEC are suitable as a guide to site prioritisation only** and should not be interpreted as accurate predictions. Detailed assessments of individual sites will require more site-specific models and extensive site characterisation and data collection. Any interpretation of results obtained using MINDEC will require a thorough understanding of the assumptions that underlie the model (see sections 2.3 and 2.4).

# 2 *B*A*C*K*G*ROU*N*D

## *2.1 Mine waste and mine waters*

Ore deposits often contain high contents of sulphide minerals. Mining and mineral processing activities give rise to large volumes of sulphide rich wastes and also create void space. Sulphide oxidation, due to exposure of waste rock and process tailings to the atmosphere, gives rise to acid mine and acid rock drainage, which is a major environmental problem. The oxidation and dissolution processes also release other potentially toxic heavy metals (e.g. Cd, Zn, Cu and Pb), which are highly soluble in acidic solutions.

The acid and high heavy metal load can represent a serious hazard for communities living downstream from a mine. Watercourses and groundwater contaminated by mine water may be used for irrigation or drinking water purposes and this can lead to ill health. For example, inhabitants of the Jintso River Valley in Japan suffered Itai-Itai disease (Kobayashi 1971) as a result of Cd poisoning. Local farmers used water with high concentrations of Zn, Cd and Pb from a nearby zinc mine to irrigate rice paddies. The rice contained Cd concentrations of around 1ppm, which led to Itai-Itai disease (Ouch-Ouch), characterised by severe bone pain. In Korea work by (Lee et al. 1999; Lee et al. 2000) has demonstrated that both Chinese cabbage and rice are accumulators of mining contamination derived-arsenic and constitute a major pathway of exposure to this metalloid for the local farming communities.

A range of pH values is observed in waters draining from metalliferous mine sites. Very low pH values may be found indicating the presence of ‘acid mine drainage’ produced by the oxidation of sulphide minerals releasing acid and heavy metals into the environment. A more neutral pH may signify that buffering has occurred due to reaction with minerals which consume acidity, e.g. calcite, while a high pH may indicate that process water rich in hydroxides has entered the system.

## *2.2 Pyrite oxidation and acid mine drainage*

Acid mine drainage (AMD) and acid rock drainage (ARD) commonly arise from the reaction of iron sulphides, notably pyrite, pyrrhotite, and arsenopyrite, with oxygen from the atmosphere. The following equations describe the processes that lead to the formation of AMD/ARD from pyrite oxidation.

$2FeS_2 + 2H_2O + 7O_2 = 2Fe^{2+} + 4SO_4^{2-} + 4H^+$ (1)

(Aqueous oxidation of pyrite ($FeS_2$) leads to the formation of ferrous iron and sulphuric acid)

The oxidation reaction of pyrite, described by Equation 1, can be subdivided as follows:

$4Fe^{2+} + 4H^+ + O_2 = 4Fe^{3+} + 2H_2O$ (2)

(Partial oxidation of ferrous to ferric iron and consumption of protons)

Ferric iron may then accept electrons, allowing further oxidation of pyrite (3), or may undergo hydrolysis (4).

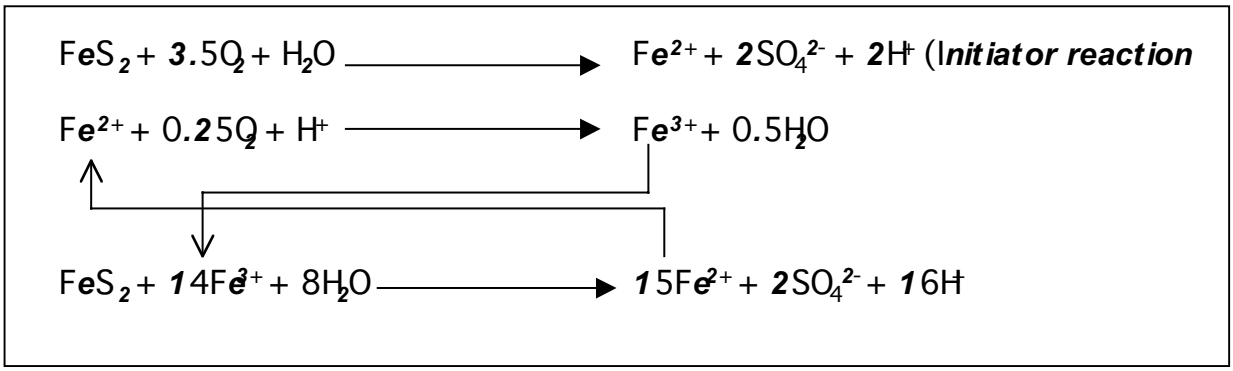
$FeS_2 + 14Fe^{3+} + 8H_2O = 15Fe^{2+} + 2SO_4^{2-} + 16H^+$ (3)

$Fe^{3+} + 3H_2O = Fe(OH)_3 + 3H^+$ (4)

Micro-organisms play a key role in the formation of AMD/ARD. The bacterium *Thiobacillus thiooxidans* oxidises sulphide minerals, whilst *Thiobacillus ferrooxidans* oxidises ferrous iron. Both *T.ferrooxidans* and *T.thiooxidans*, are chemolithotrophs that obtain energy by the oxidation of iron and sulphur respectively. The bacteria oxidise ferrous to ferric iron by a series of enzymatic reactions that occur across the cell wall leading ultimately to the reduction of oxygen to produce water. The conversion of $Fe^{2+}$ to $Fe^{3+}$ yields energy for the bacteria, however this is quantitatively small compared to the contribution of many other inorganic bacterial substrates and in order for the bacteria to achieve an adequate supply of energy from the oxidation of iron they must utilise large amounts. It has been suggested that the action of bacteria increase the rate of AMD/ARD production by a factor of 1 million.

Chemical oxidation of ferrous iron occurs rapidly at near neutral pH. When pyrite is first exposed to oxygen and water, the reaction described in Equation 1 proceeds only via a chemical pathway. The reaction produces acidic conditions under which ferrous iron is kinetically stable. *T.ferrooxidans* then catalyses the oxidation of ferrous to ferric iron. Ferric iron, which has a higher solubility in water than oxygen, reacts with pyrite (as an oxidant) to produce more ferrous and sulphate ions. This is

known as the propagation cycle (Figure 2.1), and is the root cause of acid mine drainage.




**F***igure* **2.1** *The oxidation of pyrite to form acid mine drainage*

Buffering minerals such as calcite and dolomite may reduce acidity and the heavy metal loading of mine waters. These carbonates rapidly undergo dissolution in acidic solutions (Equations 5 and 6), consuming protons and thereby raising the pH.

$CaCO_3 + 2H^+ = Ca^{2+} + H_2CO_3$ (5)
(Calcite dissolution)

$CaMg(CO_3)_2 + 4H^+ = Ca^{2+} + Mg^{2+} + 2H_2CO_3$ (6)
(Dolomite dissolution)

However, certain carbonate minerals e.g. siderite, have no buffering effect. Ferrous iron released during siderite dissolution oxidises to ferric iron and precipitates as iron oxy-hydroxide. The number of protons released during precipitation is equal to that consumed by the initial dissolution of siderite (Equations 4,7 and 8).

$FeCO_3 + 2H^+ = Fe^{2+} + H_2CO_3$ (7)
(Siderite dissolution, consumes 2 moles of protons)

$Fe^{2+} + 0.25O_2 + H^+ = Fe^{3+} + 0.5H_2O$ (8)
(Ferrous iron oxidation, consumes 1 mole of protons)

The precipitation of $Fe(OH)_3$ (ochre) results in an orange deposit commonly seen coating stream beds in mining-contaminated areas. The coating smothers and kills benthic life, but does provide sites for sorption (see below), which can act to reduce the metal loading of the water.

Aluminosilicate minerals can also act as buffers (though the kinetics of dissolution are slower than for carbonate minerals). The acidic dissolution of albite releases 1 mole of aluminium and removes 4 moles of protons (Equation 9). Subsequent dissolution of gibbsite, often observed as a white precipitate in streams contaminated by AMD/ARD, re-releases 3 moles of protons and hence 1 mole of protons is removed overall (Equation 10).

$NaAlSi_3O_8 + 4H^+ + 4H_2O = Na^+ + Al^{3+} + 3H_4SiO_4$ (9)
(Albite dissolution)

$Al^{3+} + 3H_2O = Al(OH)_3 + 3H^+$ (10)
(Gibbsite precipitation)

By raising the pH of the system, the metal loading of the water can also be reduced via:

- Precipitation of carbonates (e.g. $ZnCO_3$) and hydroxides (e.g. $Zn(OH)_2$).
- Sorption. Under acidic conditions the surface charge of ochre is positive. This attracts anions in solution e.g. arsenate and molybdenate ions. As the pH rises, the charge on the ochre surface becomes negative and thereby attracts cations in solution e.g. $Cu^{2+}$. The cations bind to the ochre surface and become immobilised in the solid phase. However, should conditions change, the metals may be released.

The composition of leachate draining from mine waste may be affected by a number of site-specific factors including the mineralogy and grain size of the minerals present, the mining and processing methods employed, the hydrogeological setting

and the prevailing climate. Mines that exploit fine-grained, sulphide-rich ore deposits, and that crush the ore to a very small size fraction, are more likely to experience acid mine drainage problems. The smaller the grain size, the greater the surface area exposed to oxidation and the greater the rate of reaction. The duration of the residence time of water in contact with ore minerals determines whether or not chemical equilibrium is achieved, or if oxidation products are flushed into surface and groundwater before *in situ* supersaturation is achieved.

## *2.3 Assumptions*

Key assumptions upon which MINDEC is based include the following:

### 2.3.1 Source Term

MINDEC considers only a single contaminant source, although there is provision to input background groundwater and surface water contaminant concentrations. If multiple contaminant sources are present these will need to be modelled separately or taken into account when setting background concentration values. The possibility that there is additional contaminant input along the transport pathway (for example, from metal-rich alluvial sediments downstream from the mine site) is not considered.

It is also assumed that representative leachate composition data are available or can be estimated. Where actual data are not available MINDEC can estimate typical leachate contaminant concentrations based on a measured or estimated pH value and simple empirical concentration-pH relationships. These concentrations may not be accurate but they are likely to be conservative, especially where the movement of water through the waste piles is rapid and water residence time in the waste is insufficient to allow equilibrium concentrations to develop.

The lifetime of pyrite in the waste pile is based on calcite mass balance considerations and is calculated on the basis that:

- the sulphate concentration value entered equals the annual average sulphate concentration of the leachate;
- all of the sulphate in the leachate originates from sulphide oxidation;
- the mine waste pile has a porosity of 20%;
- the current rate of sulphide oxidation will continue until all the pyrite has been consumed.

The lifetime of calcite in the waste pile is calculated on the basis that:

- the calcium concentration value entered equals the annual average calcium concentration of the leachate;
- all of the calcium in the leachate originates from calcite dissolution;
- the mine waste pile has a porosity of 20%;
- the current rate of calcite dissolution will continue until all the calcite has been consumed.

### *2.3.2 Pathway*

MINDEC employs a solution to the advection-dispersion equation to calculate the extent of contaminant dilution during groundwater flow. This approach assumes that flow occurs through a uniform aquifer that can be modelled as a porous medium with known aquifer properties. The possibility that fractures or highly permeable rock units can provide faster pathways for the migration of contaminants may significantly affect the accuracy of MINDEC's predictions by allowing contaminants to arrive earlier than anticipated and at higher concentrations than expected.

In general, MINDEC does not consider changes in chemistry during transport in any detail (other than those that can be approximated using a simple decay factor) as these changes are likely to be quite site-specific. In reality, this approach is likely to prove conservative since, in many cases, a number of natural attenuation and retardation processes (such as sorption, precipitation, volatilisation) may act to reduce contaminant concentrations and/or slow contaminant movement.

MINDEC does not consider transport through an unsaturated zone that may exist between the mine waste and the water table. In effect, this movement is assumed to be instantaneous and to involve no changes in contaminant concentrations.

A number of the parameters which are required as input to the model may be difficult to estimate. In general, the extent of any uncertainty in the parameter values chosen should be assessed and the likely effect on MINDEC output examined by running the model using a range of input values, i.e. by conducting a sensitivity analysis.

MINDEC only considers contaminant transport via surface water and groundwater pathways. At some sites, where wind velocities are significant, and dry, finely ground tailings are inadequately stabilised, the dispersal of potentially toxic elements through the atmosphere may be an important pathway.

### 2.3.3 *Receptor*

The human health risk calculations carried out by MINDEC consider only water consumption and do not take into account possible trace element intake from foodstuffs, e.g. derived from eating fish caught from contaminated waters and vegetables irrigated with contaminated water or grown on contaminated soil. The use of published health-related factors (reference doses, slope factor) and water quality standards involve a number of simplifications and assumptions. The reader is referred to the relevant source documentation for discussions of these issues (see for example the US EPA *Iris* database at http://www.epa.gov/iriswebp/iris/index.html)

## *2.4 Comparisons with real data*

It is important to recognise that MINDEC only calculates *annual average* contaminant concentrations at the receptor site. At any particular point in time, *actual* contaminant concentrations may differ from the MINDEC *calculated* values due to inaccuracies arising from the assumptions outlined above or due to seasonal or short-term fluctuations in concentrations which occur during the year as a result of a number of time-variant, climatically-induced factors including:

- variations in infiltration rates through the waste pile;
- variations in surface water flow rates;
- variations in groundwater flow rates; and,
- changes in chemical conditions within the waste pile and along contaminant pathways. For example, rising groundwater levels within the waste pile and/or rises in river levels may cause sudden increases in metal concentrations as highly soluble secondary minerals are dissolved and re-mobilised from the unsaturated zone. This is a particularly important mechanism in Chile for example where jarosite hydrolysis is an important mechanism of AMD/ARD generation in dried-up stream beds at the beginning of the rainy season.

# 3 THEORETICAL BACKGROUND TO MINDEC

## 3.1 Conceptual model

Site evaluation using MINDEC is achieved by considering the contaminant source term, migration pathways and potential receptors in turn (Figure 3.1). Contaminant concentrations are estimated at a chosen receptor site by estimating leachate flux and composition, dilution during surface water transport, and advection and dispersion during groundwater transport. Calculated concentration values can be compared with water quality standards and combined with water consumption data from the receptor site to calculate the risk associated with water intake.

## 3.2 Source term composition

Contaminant concentrations in leachate draining from a mine waste source may be input directly to MINDEC if these concentrations are known. Alternatively, concentrations may be estimated by MINDEC based on the leachate pH, which may itself be input directly or estimated based on a knowledge of the ore deposit host rock composition. Maximum likely concentrations of Al, Cd, Cr, Cu, Fe, Mn, Ni, Pb and Zn in leachate (for acid conditions) are determined in MINDEC on the basis of simple metal concentration – pH empirical relationships (Table 3.1). These relationships have been established by collating analyses of metalliferous mine waters reported by (Williams et al. 1996), (Williams 1995), (Williams et al. 1994), (Breward and Williams 1994), (Smedley et al. 1996), (Smedley 1996), (Smedley et al. 1998) and (Rawlins et al. 1997).

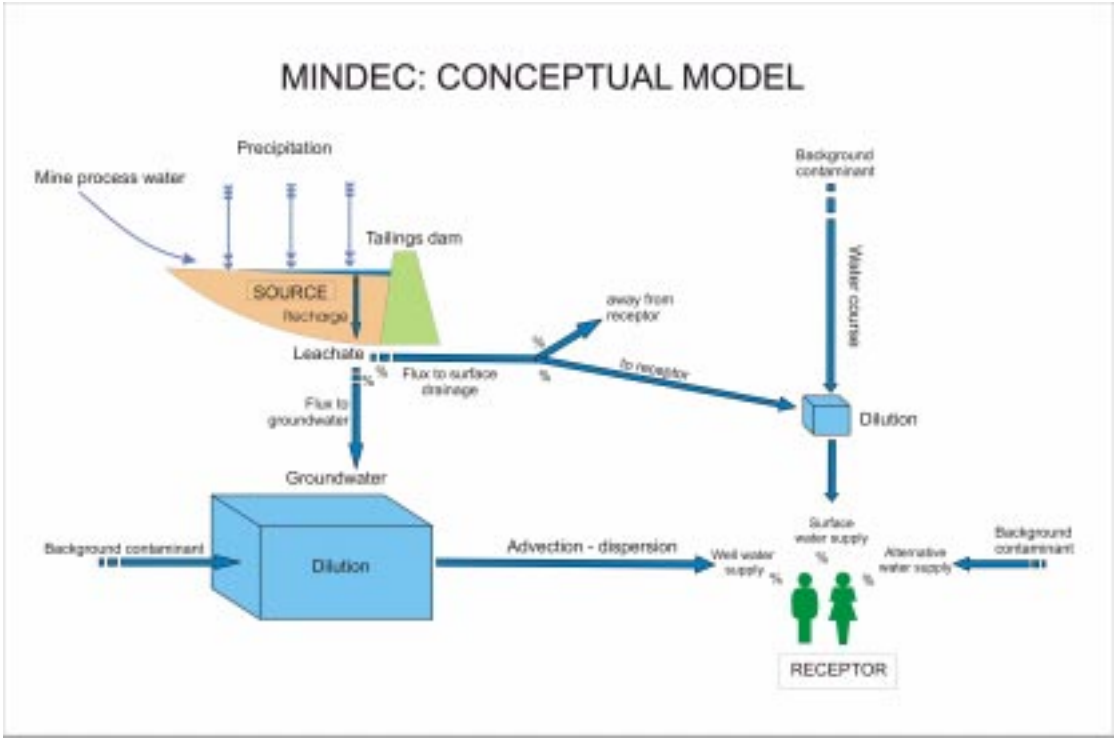



Figure 3.1: MINDEC conceptual model, showing contaminant source, surface and groundwater pathways and receptors.

Table 3.1 Equations to determine the 'maximum likely' concentrations of metals in mine waste leachate.

| **M***etal* | **E***quation* |
|---|---|
| Al | $15800\ e^{-0.92pH}$ |
| Cd | $102\ e^{-0.48pH}$ |
| Cr | $28\ e^{-0.55pH}$ |
| Cu | $4660\ e^{-0.83pH}$ |
| Fe | $281000\ e^{-1.32pH}$ |
| Mn | $3320\ e^{-0.79pH}$ |
| Ni | $21\ e^{-0.19pH}$ |
| Pb | $-0.17pH + 2$ |
| Zn | $15100\ e^{-1.01pH}$ |

### *3.3 Leachate flux*

The annual flux of leachate over the total area of the waste pile is calculated as follows:

$$L = R ((P * A_w) + T)$$

where:
L = Leachate flow rate ($m^3$ per year)
R = Recharge (as a fraction)
P = Precipitation rate (m per year)
$A_w$ = Area of waste pile ($m^2$)
T = Tailings process water volume ($m^3$ per year)

The recharge rate will depend critically on the geometry and permeability of the waste material, and on climatic factors which affect the evaporation rate from the surface of the mine waste.

Precipitation infiltrating a mine waste pile will percolate downwards towards the water table, which may lie either within or below the mine waste, at a rate which depends principally on the unsaturated zone permeability, the water-filled effective porosity and the depth to the water table. The movement of water within the unsaturated zone may also be complicated by the presence of perched water tables developed over low permeability horizons within the waste.

In general, there will be insufficient site-specific hydrogeological information to calculate travel times through the unsaturated zone. The processes of sulphide oxidation and heavy metal leaching may depend in a quite site-specific way on the availability of oxygen within the waste pile, seasonal fluctuations in this availability and the presence of minerals, principally carbonates, which act to neutralise the acidity produced.

Bearing these uncertainties in mind, MINDEC takes a conservative approach to conditions in the unsaturated zone by assuming that the source term leachate arrives at the water table instantaneously and without any solute attenuation. Essentially a saturated, piston flow, recharge process is assumed.

## *3.4 Duration of acid generation*

The mine waste module provides a very approximate indication of the potential lifetime of acid generation at the mine waste site by calculating the time required to oxidise all the pyrite in the waste pile. The long-term buffering potential of calcite in the waste pile is also assessed by calculating the time required to dissolve all the calcite in the waste pile.

During pyrite oxidation, one mole of pyrite produces two moles of sulphate:

1 mole $FeS_2$ _ 2 moles $SO_4$

and during calcite dissolution one mole of calcite produces one mole of calcium:

1 mole $CaCO_3$ _ 1 mole $Ca^{2+}$

By making a number of assumptions (see ***2.3 Assumptions***), the weathering rate of pyrite and calcite can therefore be related to leachate sulphate and calcium molar concentrations as follows:

$$R_{py} = 0.5 * [SO_4] * F_l$$
$$R_{cal} = [Ca] * F_l$$

where:
$R_{py}$ = Weathering rate of pyrite (moles/a)
$R_{cal}$ = Weathering rate of calcite (moles/a)
[Ca] = Concentration of calcium in leachate (moles/l)
$[SO_4]$ = Concentration of sulphate in leachate (moles/l)
$F_l$ = Leachate flux (l/a)

The volumes of pyrite and calcite in the waste pile can be calculated as follows:

$$V_{py} = (1-p) * V_w * C_{py}$$
$$V_{cal} = (1-p) * V_w * C_{cal}$$

where:
$V_w$ = Volume of mine waste pile (including pore space) ($m^3$)

$V_{py}$ = Volume of pyrite ($m^3$)

$V_{cal}$ = Volume of calcite ($m^3$)

$C_{py}$ = Pyrite content of waste (% by volume)

$C_{cal}$ = Calcite content of waste (% by volume)

p = Porosity of mine waste (taken as 0.2 by default)

and these volumes can be converted into weights (in moles) as follows:

$$W_{py} = 5 * 10^6 * V_{py} / 126$$

$$W_{cal} = 2.71 * 10^6 * V_{cal} / 100$$

where:

$W_{py}$ = Total weight of pyrite (moles)

$W_{cal}$ = Total weight of calcite (moles)

Hence:

$$L_{py} = W_{py} / R_{py}$$

$$L_{cal} = W_{cal} / R_{cal}$$

where:

$L_{py}$ = Pyrite lifetime (years)

$L_{cal}$ = Calcite lifetime (years)

The lifetime calculations involve a number of assumptions (see ***2.3 Assumptions***) which must be fully understood before the results can be interpreted. *The calculated lifetime values should be taken as* ***crude approximations***. They may however provide general guidance when prioritising sites.

## *3.5 Surface water transport*

Leachate from the waste pile may remain within the groundwater system or may issue at the ground surface, typically at or near the base of the steep sides of the waste pile and then enter surface drainage. The program user is required to specify the percentages of the leachate that are transported via the surface drainage and groundwater systems.

The configuration of the surface water system between the mine waste site and the receptor is difficult to generalise. MINDEC accommodates the possibility that only a

proportion of the leachate entering the surface water drainage system will flow towards the receptor site being considered. The estimation of a surface water flow rate for the purposes of the dilution calculations should be carried out bearing in mind the need to include additional tributary waterways which contribute water flow between the leachate source and the receptor.

Within the surface drainage system, dilution and attenuation processes will modify contaminant concentrations.

The diluted contaminant concentration is calculated as follows:

$$C_s = [(C_l * S * L) + (C_{bs} * R_s)] / [(S * L) + R_s]$$

where:

$C_s$ = Diluted contaminant concentration in surface water (mg/l)

$C_l$ = Contaminant concentration in leachate (mg/l)

$C_{bs}$ = Contaminant concentration in surface water upstream from mixing site (mg/l)

L = Flux of leachate from waste pile (total) (l/s)

S = Proportion of leachate entering surface water system and flowing towards the receptor

$R_s$ = Flow rate of surface water upstream from mixing site (l/s)

A flow rate value (in a variety of units) can be input or can be calculated from flow channel dimensions (depth and width) and water velocity.

Attenuation processes such as sorption and precipitation may be important in reducing contaminant concentrations in surface waters where there may be large changes in pH-Eh conditions. MINDEC adopts the conservative assumption that concentrations in surface waters are reduced only by dilution.

## *3.6 Groundwater transport*

Once leachate reaches the water table, the concentrations of dissolved trace elements will be modified by dilution with groundwater passing beneath the mine waste site and by dispersion during flow away from the site. The extent of dilution beneath the mine waste will depend on the groundwater flow rate, and the

effectiveness with which mixing between the groundwater and the contaminants occurs. MINDEC calculates the diluted contaminant concentrations beneath the mine site as:

$$C_g = [(C_l * G * L) + (C_{bg} * R_g)] / [(G * L) + R_g]$$

where:

$C_g$ = Diluted contaminant concentration in groundwater (mg/l)

$C_l$ = Contaminant concentration in leachate (mg/l)

G = Proportion of leachate entering groundwater system

L = Flux of leachate from waste pile (total) (l/s)

$R_g$ = Flow rate of groundwater upstream from mixing site (l/s)

= (k * i * A ) / 1000

where:

k = Hydraulic conductivity (m/s)

i = Hydraulic head gradient

A = Area of inflow ($m^2$)

= m * d

where:

m = mixing zone depth (m)

d = width of contaminant source perpendicular to groundwater flow (m)

MINDEC calculates the width d as the diameter of a circular mine waste pile using the value of the mine waste surface area as input by the user.

If the hydraulic head gradient is unknown then MINDEC provides an opportunity to enter the topographic gradient, since this may be much easier to measure in the absence of water level data from monitoring boreholes. MINDEC then calculates a nominal head gradient as a proportion (0.9) of the topographic gradient on the basis that head gradients in unconfined aquifers frequently reflect the surface topography. However, in rocks with a high permeability, such as karstic limestones, and/or where recharge rates are low, this approach may significantly over-estimate the head gradient. This may result in an over-estimation of contaminant dilution as a consequence of the unrealistically high flow rates predicted.

Mixing and dilution of the leachate beneath the mine waste site are considered for the purposes of the model to occur essentially instantaneously. The diluted contaminant concentrations form the source term values for groundwater transport calculations.

Dissolved contaminants will migrate down-gradient within the moving groundwater producing a plume of contamination emanating from the source. When a contaminant travels through a porous, homogeneous aquifer medium its movement is governed by the advection dispersion equation (ADE). The equation may be written as follows (Freeze and Cherry 1979):

$$\frac{\partial \mathbf{C}}{\partial \mathbf{t}} = \left[ \mathbf{D}_x \frac{\partial^2 \mathbf{C}}{\partial x^2} + \mathbf{D}_y \frac{\partial^2 \mathbf{C}}{\partial \mathbf{y}^2} + \mathbf{D}_z \frac{\partial^2 \mathbf{C}}{\partial z^2} \right] - \left[ v_x \frac{\partial \mathbf{C}}{\partial x} + v_y \frac{\partial \mathbf{C}}{\partial \mathbf{y}} + v_z \frac{\partial \mathbf{C}}{\partial z} \right]$$

where C is contaminant concentration, v is advective velocity and D is the dispersion coefficient, the subscripts x, y and z referring to the cartesian co-ordinate direction. The dispersion coefficient is defined as follows:

$$D_x = \alpha_x v_x + D^*$$

Here _ is the dispersivity and $D^*$ is the diffusion coefficient, normally ignored in calculations because of its small size compared to the product of _ and v.

The advective velocity, v is calculated from Darcy's Law:

$$\nu = \frac{k}{\eta} \frac{dh}{dx}$$

where: k = hydraulic conductivity
dh/dx = hydraulic gradient
_ = effective porosity

Based on the work of Lallemand-Barres and Peaudecerf (1978) dispersivity is usually estimated to be 10% of the flow path length and is essentially independent of aquifer type.

The ADE can also be used to estimate the transport and attenuation of contaminants that are reversibly adsorbed and result in retardation in contaminant transport rate. The ADE assumes that the porous medium is homogeneous, isotropic and saturated with fluid. An analytical solution, suitable for the situation of a mine site releasing leachate into an aquifer is given by (Domenico 1987) as:

$$C(x,\ y,\ z,\ t) = \left(\frac{C_0}{8}\right) \exp\left\{\left(\frac{x}{2\alpha_x}\right)\left[1 - \sqrt{\left(1 + \left(\frac{4\lambda\alpha_x}{v_x}\right)\right)}\right]\right\} \cdot$$

$$erfc\left[\frac{x - v_x t\sqrt{1 + \left(\frac{4\lambda\alpha_x}{v_x}\right)}}{2\sqrt{\alpha\, v_x t}}\right] \cdot$$

$$\left\{erf\left[\frac{\left(y + \frac{Y}{2}\right)}{2\sqrt{\alpha_y x}}\right] - erf\left[\frac{\left(y - \frac{Y}{2}\right)}{2\sqrt{\alpha_y x}}\right]\right\} \cdot$$

$$\left\{erf\left[\frac{\left(z + \frac{Z}{2}\right)}{2\sqrt{\alpha_z x}}\right] - erf\left[\frac{\left(z - \frac{Z}{2}\right)}{2\sqrt{\alpha_z x}}\right]\right\}$$

where: $C_0$ is the initial concentration and _ is the decay constant. This equation is readily manipulated in a spreadsheet and has been implemented within MINDEC.

### *3.7 Contaminant attenuation and retardation*

MINDEC has provision for inputting attenuation (biodegradation/decay) and retardation factors due to sorption for groundwater transport but the program does not otherwise consider contaminant attenuation processes other than dilution.

Sorption is determined experimentally by measuring the amount of solute retained by a solid in batch experiments. The sorption may be described as a linear relationship between the sorbed concentration $C^*$ and the solute concentration C, (see Figure 3.2) such that:

$C^* = K_d.C$

where $K_d$ is the distribution coefficient.

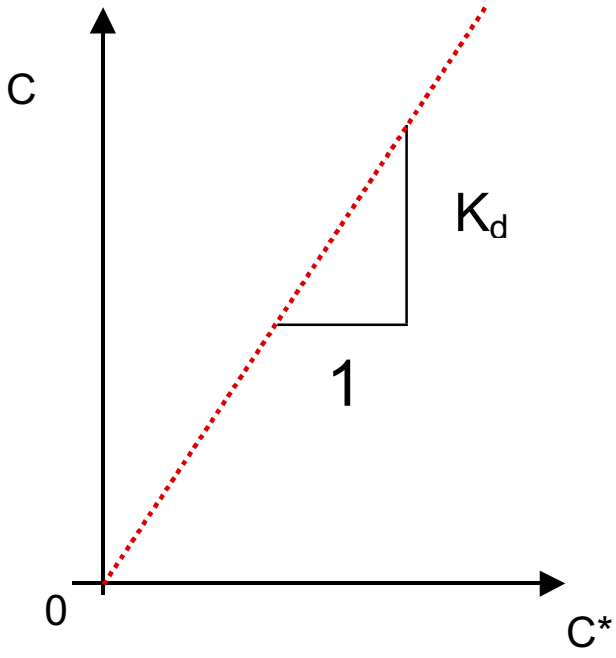



Figure 3.2 The linear isotherm

The retarded advective velocity, $v_c$, is then calculated using the following equations:

$$r_f = 1 + \frac{\rho_d}{\eta} .K_d$$

$$v_c = \frac{v_x}{r_f}$$

Where: $r_f$ is the retardation factor

$\eta$ is the effective porosity

$\rho_d$ is the dry bulk density

$v_x$ is the advective velocity

## *3.8 Water usage*

In order to evaluate the risks to the health of water consumers at the receptor site MINDEC considers three possible sources for drinking water:

- Groundwater (potentially contaminated by mine waste leachate)
- Surface water (potentially contaminated by mine waste leachate)
- Water from some other source (such as rain water or water not potentially contaminated by mine waste)

Some careful interpretation of transport pathways may be required in order to establish appropriate percentage values for these various sources, since some water may arrive at the receptor via a mixed surface/groundwater path. For example, water abstracted from a well immediately adjacent to a river might contain contaminants that have been transported largely within surface water before being drawn into the well. It would therefore be more appropriate for MINDEC to consider this water as surface water rather than groundwater since groundwater transport calculations would over-estimate travel times and miscalculate the extent of any dilution and dispersion.

Similarly, careful consideration should be given to the possibility that contaminants might reach the receptor after migrating first through groundwater and then discharging into surface water.

An effective combined concentration at the receptor site is calculated by MINDEC based on the relative volumes of water consumed from these three sources, as follows:

$$C_{com} = (D_g * C_g) + (D_s * C_s) + (D_a * C_a)$$

where:
$C_{com}$ = Effective combined concentration (mg/l)
$C_g$ = Concentration in groundwater (mg/l)
$D_g$ = Volume of groundwater consumed as proportion of total
$C_s$ = Concentration in surface water (mg/l)
$D_s$ = Volume of surface water consumed as proportion of total
$C_a$ = Concentration in alternative source water (mg/l)

$D_a$ = Volume of alternative source water consumed as proportion of total

The combined concentrations can be compared with water quality standards and/or combined with water consumption data to calculate hazard quotients for potentially toxic elements and a carcinogenic risk for arsenic.

### *3.9 Risk assessment*

Measured or estimated contaminant concentrations in leachate at the source and at the receptor site can be compared with water quality standard data. The World Health Organization, European Union and United Kingdom drinking water standards are provided as default data sets in MINDEC. Alternatively the user can input any alternative water quality standard data sets. A Water Quality Standard (WQS) Exceedance Index is calculated as the highest of the ratios of the actual or estimated contaminant concentrations to the respective WQS values for each of the elements under consideration. The combined concentration ($C_{com}$) for any element is calculated as follows:

$$C_{com} = (C_{gr} . g + C_s . s + C_{alt} . a) / 100$$

where: $C_{gr}$ = Concentration in groundwater (mg/l)
$C_s$ = Concentration in groundwater (mg/l)
$C_{alt}$ = Concentration in groundwater (mg/l)
g = % groundwater consumed
s = % surface water consumed
a = % alternative source water consumed

If water quality criteria are not met then a deterministic risk assessment can be carried out.

Risk assessment ***is a*** formalised framework enabling determination of the relationship between the predicted exposure /concentration of a given substance or substances and predicted adverse effects on human health. Hazard and risk are frequently confused: they are not synonymous. At the most basic level hazard equates to danger, and in the risk assessment context a hazard exists if a potential exists to cause harm. Conversely, risk is the likelihood of an adverse event occurring in response to a hazardous situation.

A risk assessment is subdivided into three stages, essentially following the classical source – pathway – receptor model. They are:

1. Hazard identification, i.e. the contaminated groundwater and the metals present.
2. Exposure assessment, i.e. determination of contaminant concentrations at the receptor.
3. Dose – response assessment based on contaminant ingestion by the receptor.

The preliminary step in exposure assessment is the construction of a conceptual model that represents the exposure pathways. In MINDEC the exposure pathways are via the consumption of surface and contaminated groundwater.

The dose assessment is achieved by estimating total environmental exposure to a particular hazardous compound identified in the source. Elements derived from mine waste either constitute a toxic hazard or in the case of arsenic both a toxic and a carcinogenic hazard.

### **3.9.1** *Toxic* **R***isk*

The general practice is to assume that a toxic chemical has a threshold below which toxic effects do not occur. Toxic hazard estimates are expressed relative to a reference dose concentration. The reference dose is an exposure that can occur over a prolonged period without ill effect. Risk estimates are based on a comparison of actual exposure to this reference dose (Rfd) for the particular chemical involved and a Hazard Quotient (dimensionless) is calculated as follows:

$$HQ = \frac{ADD}{Rfd}$$

where: ADD is the average daily dose. The units of the ADD and Rfd are mg/kg of body weight per day. A toxic risk exists for HQ>1.

The ADD is calculated as follows:

$$ADD = \frac{C \cdot IR}{BW} \cdot \frac{EF}{365}$$

where C is the contaminant concentration (mg/l), IR is the ingestion rate of water (l/day), BW is body mass (kg), EF is the exposure frequency (days/year).

The MINDEC model uses the Rfd values given in Table 3.1. The Rfd is compound specific and updates of these values may be obtained from the US EPA I*R*IS database.

Table 3.1 Reference doses used in MINDEC

| ***Metal*** | ***RfD*** |
|---|---|
| As | 0.0003 |
| Cd | 0.0005 |
| Cr | 0.005 |
| Hg | 0.0001 |
| Ni | 0.02 |
| Zn | 0.3 |
| Mn | 0.014 |

### *3.9.2 Carcinogenic Risk*

Carcinogenic compounds differ from systemic toxic compounds in that there is no lower limit for the existence of cancer risk. Carcinogenic risk is calculated as follows:

$$risk = 1 - \exp(-SF \cdot LADD)$$

where: SF is the slope factor that is derived from laboratory dose-response experiments, assumed to be linear in the low dose range. It should be remembered that this equation calculates the increased risk of getting cancer and not of dying from cancer. The US EPA considers an increased risk of cancer of 1 in 1000000 as significant.

The LADD is the lifetime average daily dose and is calculated from the ADD as follows:

$$LADD = ADD \cdot \frac{ED}{LE}$$

where: ED is the exposure duration in years and LE is the average life expectancy.

Although risk assessment involves the application of seemingly trivial mathematical equations, problems arise in their parameterisation, and a detailed knowledge of exposure factors is required in order to make the calculations useful. The following table (Table 3.2) indicates the information required in order to parameterise the risk assessment module of MINDEC.

*Table* **3.2 D***ata requirements for the risk assessment model*

| ***Data Type*** | ***Data Requirement*** |
|---|---|
| **D***emographic* **D***ata* | **L***ife expectancy, body mass* |
| **E***xposure* **D***ata* | **E***xposure duration, frequency of exposure, water ingestion rate* |

The US EPA have recently published a revised issue of the Exposure Factors Handbook, now available on CD (USEPA 1999) and also on the internet at http://www.epa.gov/nceawww1/exposfac.htm, and reference should be made to this for further background information.

# 4 USING MINDEC

## 4.1 Software requirements

MINDEC is programmed in Visual Basic for Applications (VBA) and runs under Microsoft Excel 97 / Excel 2000 but will not run under pre-97 versions of Excel. Either Microsoft Excel 97 or Excel 2000 is therefore required in order to run MINDEC.

MINDEC is compatible with Windows 95, Windows 98, Windows NT version 4, and Windows 2000.

## 4.2 International issues

MINDEC has been tested with English and Spanish-language versions of Excel 97 under English and Spanish Windows Regional Settings. It has not been tested with other language settings and will display an advisory message on starting up for the first time if it detects a non-English language environment.

The user should be aware that, although MINDEC on-screen text is displayed in the English language, default VBA message boxes which display during program execution contain buttons with captions which will be automatically displayed in the language appropriate to the user's version of Windows.

## 4.3 Hardware issues

### 4.3.1 *Minimum requirements*

Recommended minimum requirements are for a 150MHz Pentium PC with 32Mb RAM. Using a faster PC will speed up screen loading and unloading. Operating the program with inadequate video RAM may cause 'Out of memory' errors. The program requires 6Mb of hard disk space for installation.

### 4.3.2 *Screen size*

MINDEC screens are modal, which means that they cannot be minimised, maximised or otherwise re-sized. A usable screen area sufficiently large to display the fixed-size screens is therefore required. In order to achieve this, a screen resolution of at least 800 x 600 should be available with a nominal screen size of at least 15 inches. (The screen resolution can be checked from the Windows Control Panel, if required). On

start-up MINDEC interrogates the system hardware of the computer that it is running on and will display a warning message and then abort the program if the available screen area is insufficiently sized.

## 4.4 Installation

MINDEC can be installed by running the executable installation file ***mindec setup.exe***. MINDEC consists of the following files:

| | |
|---|---|
| Mindec.xls | MINDEC Excel/VBA application file |
| Refdata.xls | Water quality standard reference data file |
| Mdechlp.hlp | MINDEC on-line help file |
| Example.mdc | An example scenario file |
| readme.txt | Text files |
| Conditions.txt | |

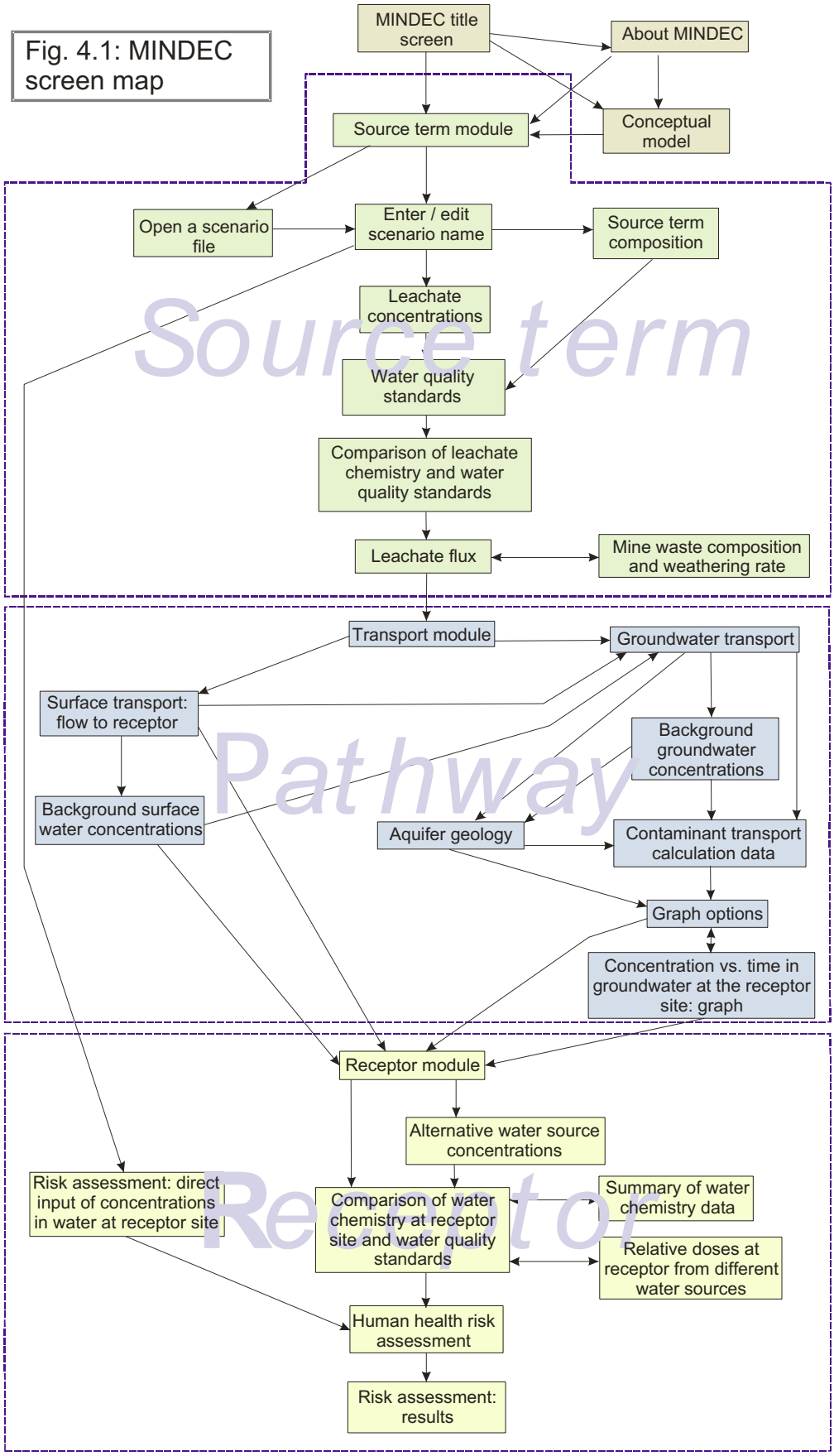
To run the program, open Mindec.xls and then wait while MINDEC loads. This may take some time. If a message referring to running macros appears, choose to accept macros.

## 4.5 MINDEC program screens

### 4.5.1 Introduction

MINDEC presents a series of graphical screens to the user. The screens have been designed to focus on different parts of the source-pathway-receptor linkage and to prompt the user for required input data in a logical sequence (see Figure 4.1). The screens are described below in alphabetical order.

Fig. 4.1: MINDEC screen map


MINDEC title screen
About MINDEC
Source term module
Conceptual model
Open a scenario file
Enter / edit scenario name
Source term composition
Leachate concentrations
Water quality standards
Comparison of leachate chemistry and water quality standards
Leachate flux
Mine waste composition and weathering rate
Source term
Transport module
Groundwater transport
Surface transport: flow to receptor
Background groundwater concentrations
Background surface water concentrations
Aquifer geology
Contaminant transport calculation data
Graph options
Concentration vs. time in groundwater at the receptor site: graph
Pathway
Receptor module
Alternative water source concentrations
Risk assessment: direct input of concentrations in water at receptor site
Comparison of water chemistry at receptor site and water quality standards
Summary of water chemistry data
Relative doses at receptor from different water sources
Human health risk assessment
Risk assessment: results
Receptor

### 4.5.2 A*lternative water source concentrations*

Enter contaminant concentrations as measured in the alternative source water.

Alternative water concentrations can only be entered for elements for which leachate concentrations have been entered (or calculated by MINDEC).

Note: If a concentration value is not entered for a particular element then the concentration for that element will be assumed to be zero.

Enter all concentrations in mg/l.

### 4.5.3 A*quifer Geology*

Select the lithology that best describes the groundwater pathway between the source and the receptor from the drop-down menu. Only one lithology can be selected. Appropriate values for the hydraulic conductivity and porosity of the chosen lithology are then applied from MINDEC's database (Table 4.1). To enter values for the hydraulic conductivity and porosity directly, press the 'Advanced' button.

Other parameters required for contaminant transport calculations are given default values. To view and/or change any of these values, press the 'Advanced' button.

Use the option buttons to indicate the relative importance of matrix / fracture flow. If fracture flow is significant or predominant then the user is warned that the groundwater transport calculations may be invalid.

Table 4.1 Representative values of porosity and hydraulic conductivity.

| **L***ithology* | **H***ydraulic conductivity* **[***m/s***]** | P*orosity* **[%]** |
|---|---|---|
| *Gravel* | 3.0E-03 | 30 |
| *Coarse sand* | 7.3E-05 | 35 |
| **M***edium sand* | 2.1E-05 | 35 |
| **F***ine sand* | 6.3E-06 | 40 |
| *Silt* | 1.4E-07 | 45 |
| *Till* | 1.4E-09 | 50 |
| *Clay* | 2.2E-10 | 50 |
| **K***arstic limestone* | 1.4E-04 | 30 |
| **L***imestone* | 7.7E-08 | 10 |
| *Sandstone* | 4.2E-08 | 20 |
| *Siltstone* | 3.7E-10 | 10 |
| *Shale* | 1.4E-11 | 10 |
| P*ermeable basalt* | 8.9E-05 | 25 |
| *Basalt* | 2.9E-09 | 5 |
| **F***ractured igneous and metamorphic rocks* | 1.5E-06 | 10 |
| **U***nfractured igneous and metamorphic rocks* | 2.4E-12 | 1 |
| *Weathered granite* | 1.3E-05 | 5 |
| *Weathered gabbro* | 1.4E-06 | 5 |

Data from (Domenico and Schwartz 1998) and (Freeze and Cherry 1979).

### **4.5.4** *Background Groundwater Concentrations*

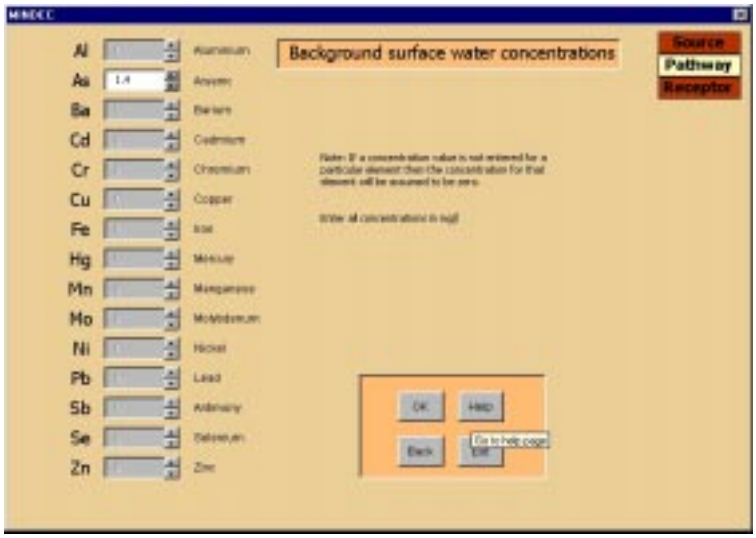
Enter contaminant concentrations as measured in groundwater upstream from the contamination source under consideration.

Background concentrations can only be input for elements for which leachate concentrations have been entered (or calculated by MINDEC).

Note: If a concentration value is not entered for a particular element then the concentration for that element will be assumed to be zero.

Enter all concentrations in mg/l.

### **4.5.5** *Background Surface Water Concentrations*



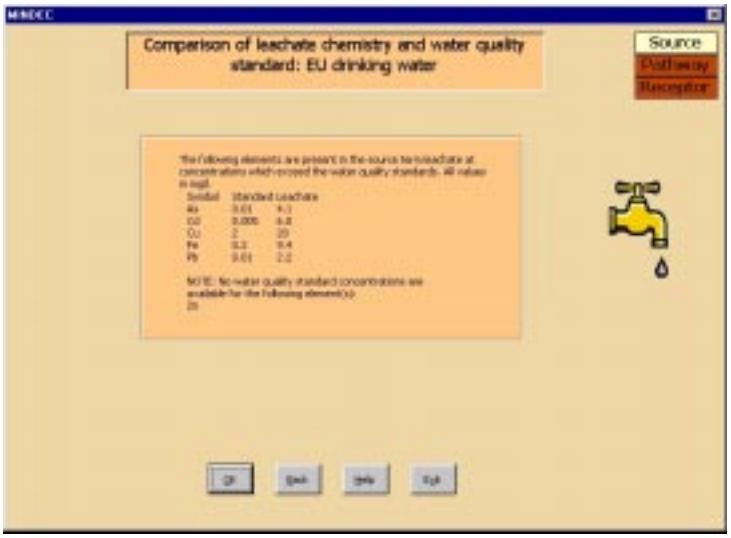

Enter contaminant concentrations as measured in surface water upstream from the site of mixing with leachate.

Background concentrations can only be input for elements for which leachate concentrations have been entered (or calculated by MINDEC).

Note: If a concentration value is not entered for a particular element then the concentration for that element will be assumed to be zero.

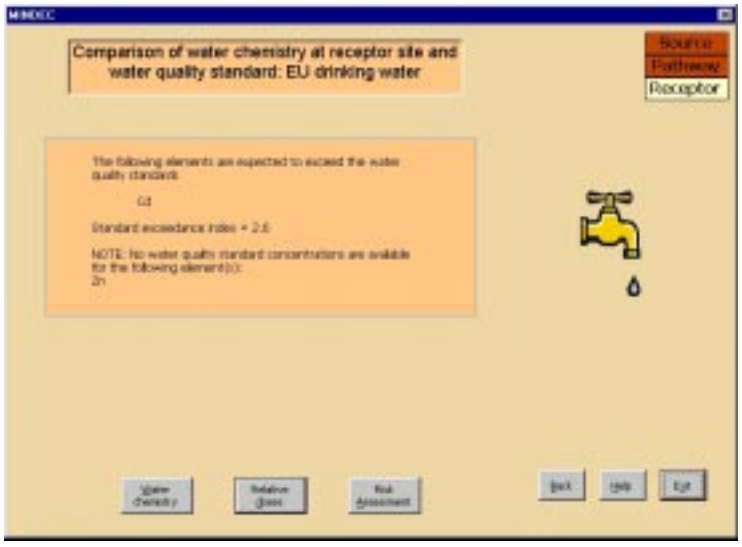
Enter all concentrations in mg/l.

### **4.5.6** *Comparison of* **L***eachate Chemistry and Water* **Q***uality Standard*




Leachate concentration data are compared with the water quality standard (WQS) data set previously selected. Concentrations that exceed the water quality standard data are displayed on-screen.

### **4.5.7** *Comparison of Water Chemistry at* **R***eceptor Site and Water* **Q***uality Standard*



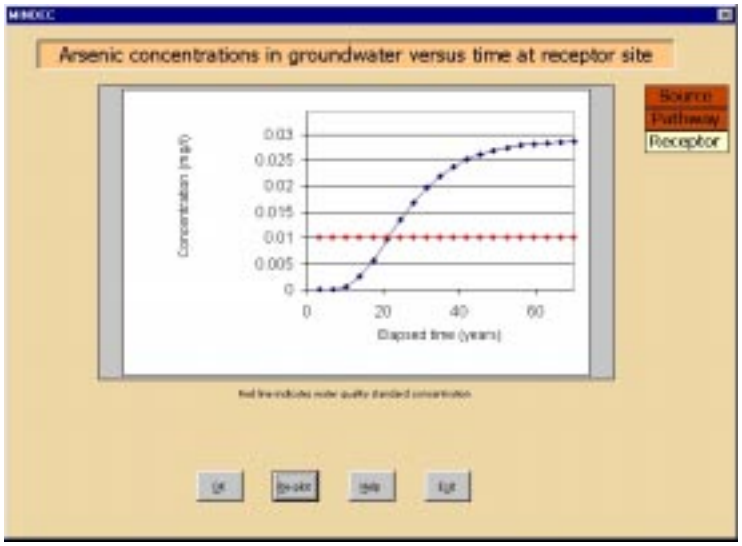

Calculated combined source contaminant concentrations at the receptor are compared with the water quality standard (WQS) data set previously selected by calculating (contaminant concentration / standard) ratios for each element for which suitable data are available. The highest of these calculated ratios is quoted as the *WQS exceedance index* for the modelled scenario.

Calculated concentration data can be viewed by clicking on the 'Summary data' button.

Calculated relative doses (as % of total dose) from different water sources for each element of interest can be viewed by clicking on the 'Relative doses' button.

Click on 'Risk assessment' to carry out a human health risk assessment based on the calculated concentrations.

### **4.5.8** *Concentrations vs Time in Groundwater at the* **R***eceptor Site*




Contaminant concentrations are calculated using a 3-dimensional solution to the advection-dispersion equation and the source term and aquifer property data entered into the model. It is assumed that the concentrations cannot fall below the groundwater background concentrations that have been entered into the model.

By default, the time scale (x-axis) extends from zero to twice the age of the source term (as input by the user). Zero represents the time at which the leachate first entered the groundwater system. No account is taken of the time taken by the leachate to migrate through the unsaturated zone between the source term and the groundwater. The indicated time therefore provides a conservative estimate of groundwater travel times. To adjust the time and concentration ranges shown, or to select a different element to plot, press the 'Re-plot' button. When comparing re-plotted graphs attention should be paid to the concentration scale (y-axis), as this may adjust automatically to display most effectively the values to be plotted.

If an appropriate water quality standard (WQS) concentration is available from the WQS data set selected previously, this value is plotted as a red line so that this concentration can be compared with the predicted groundwater concentrations.

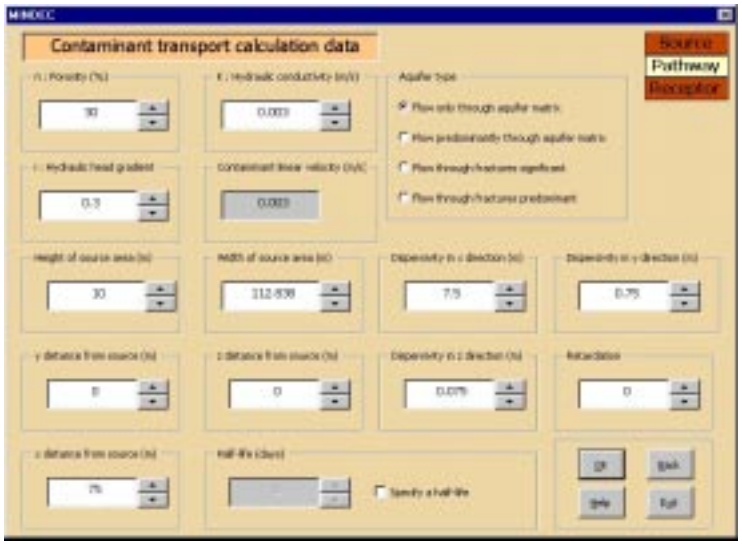
The displayed graph may show concentrations rising with time as a plume of contaminated groundwater arrives at the receptor or concentrations which are unchanged with time. Constant concentrations may indicate that:

- insufficient time has elapsed for the contaminated groundwater to reach the receptor; or,
- background groundwater contaminant concentrations exceed leachate contaminant concentrations; or,

- contaminant present in leachate has been massively diluted by groundwater flow and therefore no significant contaminant plume exists at the location of the receptor.

***WARNING: the concentrations shown are based on calculations that assume flow through a porous medium. If fracture flow is significant, then the contaminant may arrive at the receptor at an earlier time and at higher concentrations than those indicated.***

### **4.5.9** *Contaminant Transport Calculation* **D***ata*




If required, the user can input all of the data required for groundwater contaminant transport calculations rather than allow MINDEC to adopt default values. The parameters that can be set by the user are as follows:

**A***ge* **(***years***)**: age of source term.

P*orosity* **(%)***:* aquifer effective porosity.

**H***ydraulic conductivity* **(***m/s***)***:* aquifer hydraulic conductivity.

**H***ydraulic head gradient:* the hydraulic head gradient along the groundwater pathway.

*Contaminant average linear velocity* **(***m/s***)***:* the velocity is calculated automatically from the porosity, hydraulic conductivity and hydraulic head gradient values. Porosity and velocity data must be entered in the appropriate boxes before continuing to the next screen.

**H***eight of source area* **(***m***)***:* this refers to the height of the notional cell of groundwater beneath the contaminant source (mine waste) within which leachate-groundwater mixing occurs. Mixing within this cell is assumed to be complete and effectively instantaneous. The cell acts as the source term for groundwater contaminant transport calculations. By default the height is taken to be 10m.

*Width of source area* **(***m***)***:* this refers to the height of the notional cell of groundwater beneath the contaminant source (mine waste) within which leachate-groundwater mixing

occurs. A default value for the width is calculated from the area of the waste (as entered by the user) and an assumed circular shape for the waste pile.

**D***ispersivity* **(***m***)** *in x-direction:* a measure of the extent of dispersion (mixing) of the contaminant in the horizontal plane and parallel to the direction of flow. By default the dispersivity in the x-direction is set to 0.1 * x-distance from source.

**D***ispersivity* **(***m***)** *in y-direction:* a measure of the extent of dispersion (mixing) of the contaminant in the horizontal plane and perpendicular to the direction of flow. By default the dispersivity in the y-direction is set to 0.01 * x-distance from source.

**D***ispersivity* **(***m***)** *in* **z***-direction:* a measure of the extent of dispersion (mixing) of the contaminant in the vertical direction. By default the dispersivity in the z-direction is set to 0.001 * x-distance from source.

**R***etardation:* a retardation factor describing the retardation of a contaminant relative to groundwater movement (most commonly due to sorption): the ratio of the average linear groundwater velocity to the average velocity of the contaminant. Note that the retardation factor will be applied equally to all the elements included in the scenario.

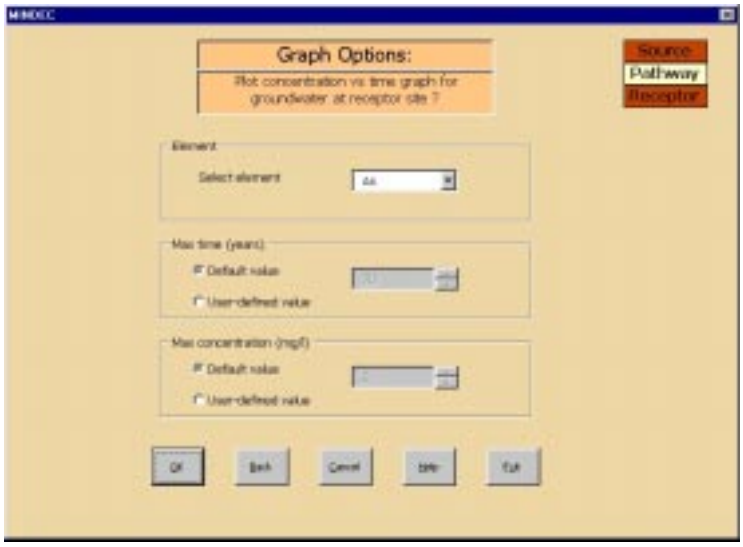
*x-distance from source* **(***m***)***:* the distance between the source and the receptor measured in the horizontal plane parallel to the main direction of groundwater flow.

*y-distance from source* **(***m***)***:* the distance between the source and the receptor measured in the horizontal plane perpendicular to the main direction of groundwater flow.

**z***-distance from source* **(***m***)***:* the vertical distance between the source and the receptor.

**H***alf-life* **(***days***)***:* half-life describing decay of the element of interest. Note that the half-life will be applied equally to all the elements included in the scenario. It may therefore be best to model elements one-by-one if decay is to be included in the calculations. To enter a half-life, check the 'Specify a half-life' box and enter a half-life in days.

### **4.5.10** *Graph* ***O****ptions*

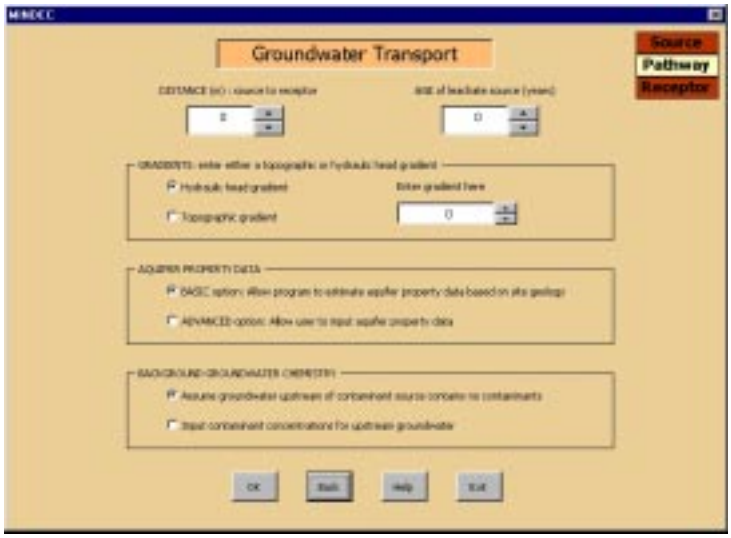



To display a graph of changes in contaminant concentration with time at the receptor site, select the appropriate element and enter maximum time and concentration values (or accept the default values). The default time value is set at twice the age of the source term. The default concentration value is set to display all of the available data.

Note - only elements for which data are available are selectable from the drop-down menu.

To proceed without plotting a graph, press the 'Cancel' button.

### **4.5.11** *Groundwater Transport*




#### **D***istance*

Enter the straight-line source to receptor distance in metres.

#### **A***ge of* **L***eachate Source*

Enter the age of the leachate source in years.

#### *Gradient*

Enter a value for the hydraulic gradient (x/y) if this is known or can be estimated.

If the hydraulic head gradient is unknown then MINDEC provides an opportunity to enter the topographic gradient, since this may be much easier to measure in the absence of water level data from monitoring boreholes. MINDEC then calculates a nominal head gradient as a proportion (0.9) of the topographic gradient on the basis that head gradients in unconfined aquifers frequently reflect the surface topography. However, in rocks with a high permeability, such as karstic limestones, and/or where recharge rates are low, this approach may significantly over-estimate the head gradient. This would cause both the extent of dilution of contaminants beneath the waste site and contaminant velocities to be over-estimated. As a consequence, contaminants might reach the receptor at a higher concentration than predicted although actual travel times might be longer than those estimated. Therefore, if the nominal head gradient (based on the topographic gradient) is considered to be unrealistic, the user should enter a better estimate of the head gradient even if accurate data are not available.

#### **A***quifer* P*roperty* **D***ata*

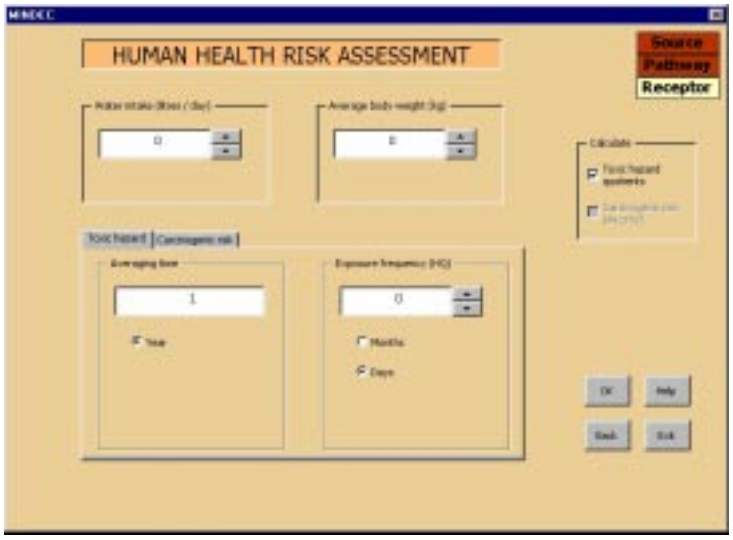
Select either the

*B***A***SIC* option: in which case porosity and hydraulic conductivity values are taken from MINDEC's internal database of values based on a lithology specified by the user in the

following screen. Other parameters for groundwater transport calculations are set to default values.
or the **ADVA***NC***ED** option: in which case all parameters required for groundwater transport calculations can be set by the user.

Select the appropriate option to take into account background, groundwater, contaminant concentrations or to assume that the groundwater is uncontaminated upstream of the source being modelled.

### 4.5.12 Human Health Risk Assessment




**Data entry**

(1) Enter the following water consumer (receptor) data in the appropriate boxes:

*Water intake* (*litres per day*)
**A***verage body weight* (*kg*)

(2) For the toxic hazard calculations, click on the grey 'Toxic hazard' tab and enter:

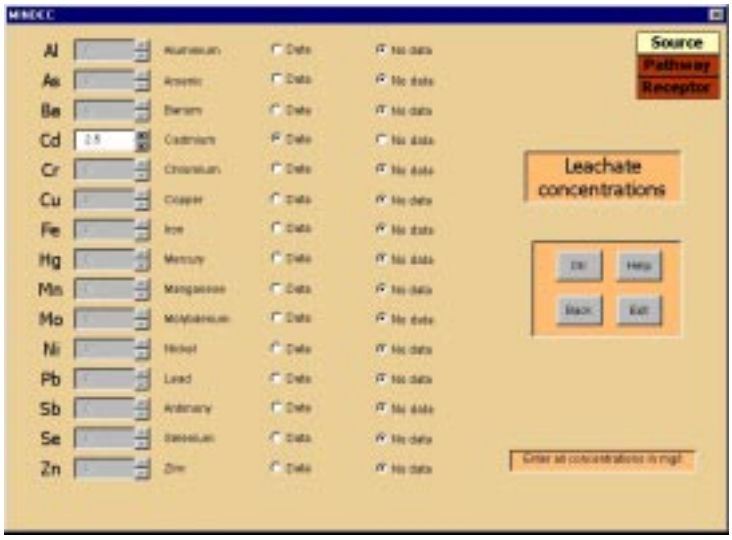
**E***xposure frequency:* that part of the averaging time (365 days) during which the receptor has been exposed to contaminants.

(3) For the carcinogenic risk calculation, click on the grey 'Carcinogenic risk' tab and enter:

**L***ifetime expectancy:* the time span over which an average daily dose of each contaminant of interest is to be calculated.
**E***xposure time*: that part of the lifetime during which the receptor has been exposed to the carcinogen.

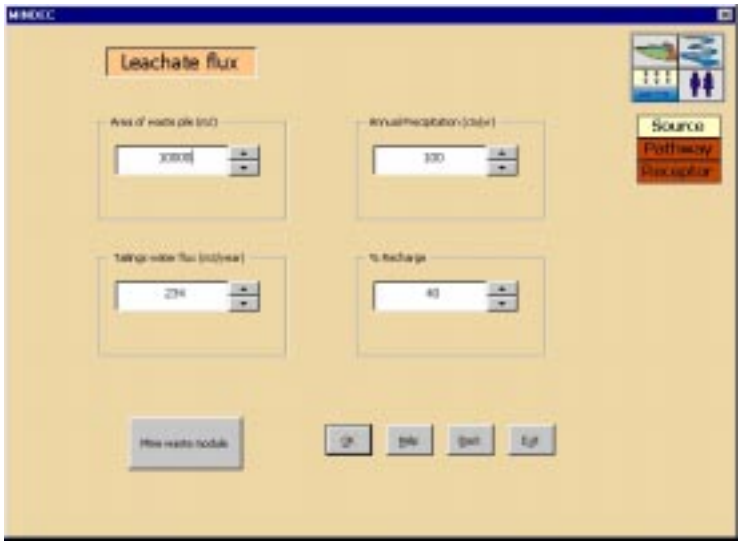
Note that the check boxes in the ‘Calculate’ frame are for information only and cannot be re-set by the user. . The carcinogenic risk calculation is not available if data for arsenic have not been entered. The toxic hazard averaging time is set to 1 year and cannot be adjusted by the user.

### 4.5.13 L*eachate Concentrations*




Enter the leachate concentrations (in mg/l) for elements for which data are available, by pressing the 'Data' option button to activate the appropriate data input box. Then type the concentration value into the box or use the up/down spin buttons to scroll to the required value.

### 4.5.14 L*eachate* F*lux*

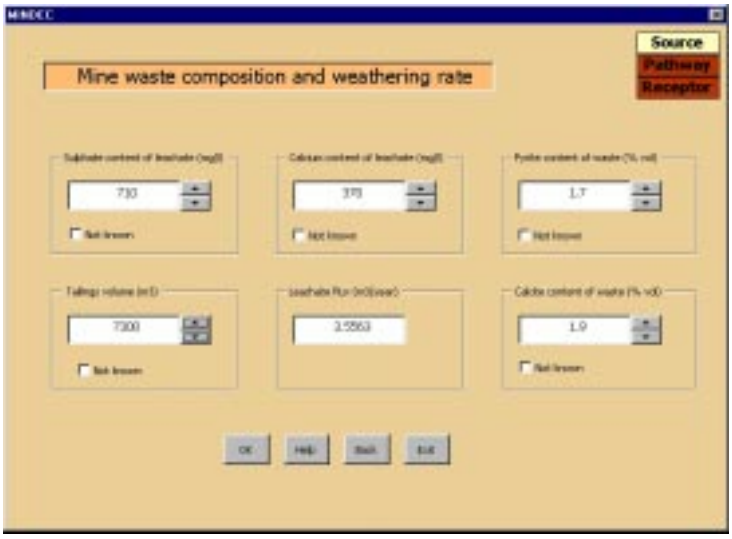



The leachate flux from a mine waste source is calculated over the total area of the waste pile. The user must provide values for precipitation rate (cm/yr) and area of the waste pile ($m^2$). The recharge rate will depend critically on the permeability of the waste material, and on climatic factors which affect the evaporation rate from the surface of the mine waste.

The 'Mine waste module' button allows the user to calculate the potential lifetime of acid generation at the site.

Click on the navigation images in the top-right corner of the window to move directly backwards to the MINDEC Source Term screen if required. Note that it is not possible to jump forwards to the Transport or Receptor screen.

### 4.5.15 M*ine waste composition and weathering rate*




The mine waste module provides a very approximate indication of the potential lifetime of acid generation at the site by calculating the time required to oxidise all the pyrite in the waste pile. The long-term buffering potential of calcite in the waste pile is also assessed by calculating the time required to dissolve all the calcite in the waste pile.

Enter the appropriate data (where available) after activating the corresponding data input boxes by un-checking the 'Not known' boxes.

Calculation of a pyrite lifetime requires a leachate flux, a mine waste volume, a waste pyrite content and a leachate sulphate concentration.

Calculation of a calcite lifetime requires a leachate flux, a mine waste volume, a waste calcite content and a leachate calcium concentration.

The leachate flux is displayed on this screen but the value can only be adjusted by returning to the 'Leachate flux' screen.

The lifetime calculations involve a number of assumptions that must be fully understood before the results can be interpreted.

#### P*yrite lifetime*

The lifetime of pyrite in the waste pile is calculated on the basis that:

- the sulphate concentration value entered equals the annual average sulphate concentration of the leachate;
- all of the sulphate in the leachate originates from sulphide oxidation;
- the current rate of sulphide oxidation will continue until all the pyrite has been consumed.

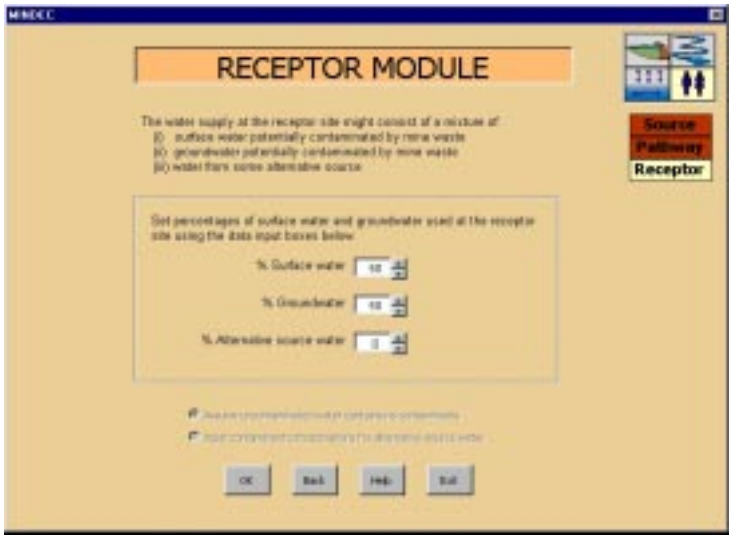
### *Calcite lifetime*

The lifetime of calcite in the waste pile is calculated on the basis that:

- the calcium concentration value entered equals the annual average calcium concentration of the leachate;
- all of the calcium in the leachate originates from calcite dissolution;
- the current rate of calcite dissolution will continue until all the calcite has been consumed.

The calculated lifetime values should be taken as crude approximations. They may however provide general guidance when comparing sites.

### 4.5.16 R*eceptor* M*odule*



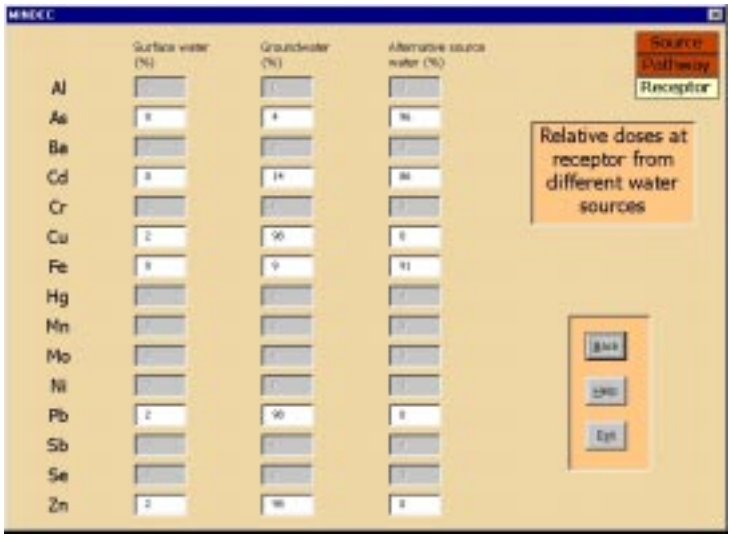

Leachate from the waste pile may remain within the groundwater system or may issue at the ground surface, typically at or near the base of the steep sides of the waste pile and then enter surface drainage. The program user is therefore required to specify the percentages of the leachate which are transported via the surface drainage and groundwater systems. MINDEC considers the possibility that a water consumer (the receptor) ingests water from a variety of water sources:

- Surface water potentially contaminated by the source under consideration;
- Groundwater abstracted from a well / borehole, potentially contaminated by the source under consideration; and
- Water from some alternative source (possibly uncontaminated)

Enter appropriate values into the boxes and then press 'OK'.

Click on the navigation images in the top-right corner of the window to move directly backwards to the MINDEC source term, leachate flux or transport screens if required.

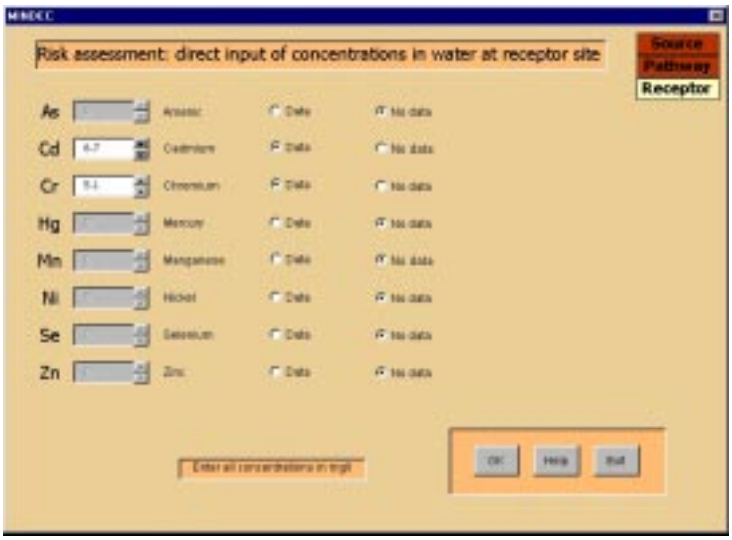
### 4.5.17 R*elative doses at receptor from different water sources*




This screen presents a summary of calculated relative doses to which the receptor is exposed through consumption of surface water, groundwater and water from an alternative source. Doses are calculated from estimated concentrations ion the different waters and the relative volumes of these waters consumed by the receptor.

The relative doses should be interpreted bearing in mind the large number of assumptions that are inherent within the modelling process.

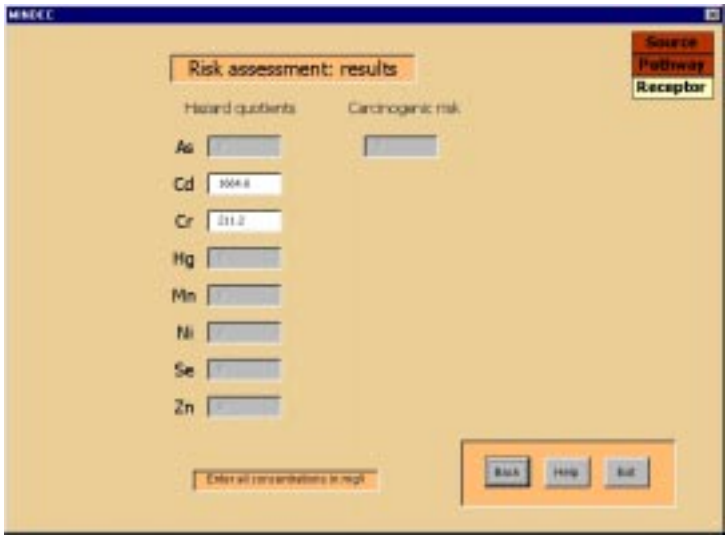
### 4.5.18 R*isk assessment: direct input of concentrations in water at receptor site*




If analytical data are available for the water at the receptor site then enter the data in the appropriate boxes and press the 'OK' button to carry out a human health risk assessment.

Data can only be entered for those elements for which reference doses have been established (As, Cd, Cr, Hg, Mn, Ni, Se, Zn), since these values are required for toxic hazard quotient calculations.

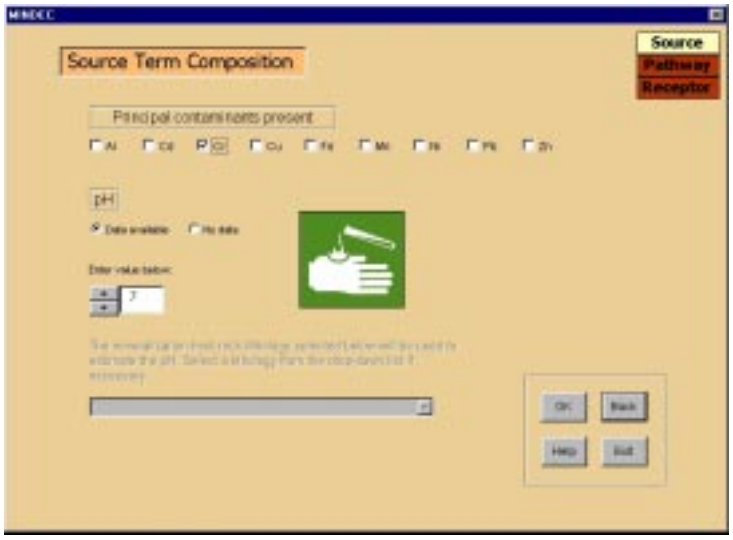
### 4.5.19 R*isk assessment: results*




Calculated hazard quotients and a carcinogenic risk factor (for arsenic) are displayed.

Press ‘Back’ to return to the main Risk Assessment screen.

### **4.5.20** *Source Term Composition*

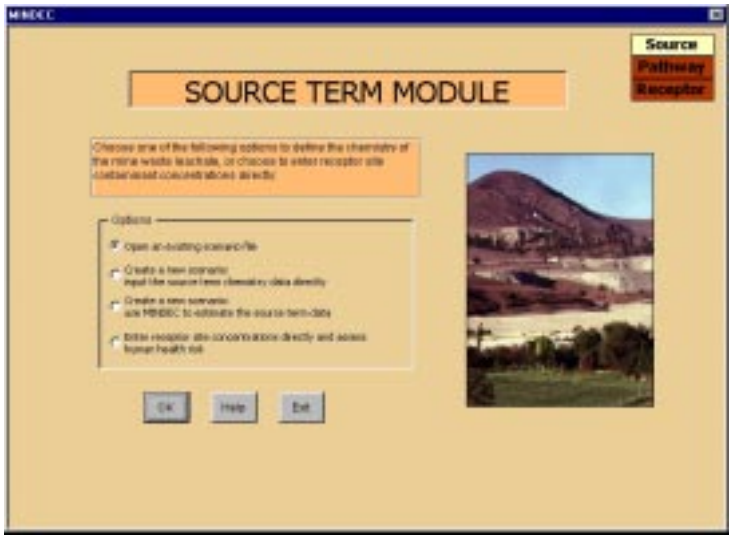



Elements/ metals likely to be present in the mine waste leachate should be selected using this screen.
Either: enter a measured leachate pH; or, if this is not available, select a mineralisation host rock type from the drop-down menu to allow MINDEC to estimate the pH.

In the latter case, the estimated pH is shown in a message box and the user then has an opportunity to accept or reject this value.

A measured or estimated pH value is required for MINDEC to estimate a leachate composition.

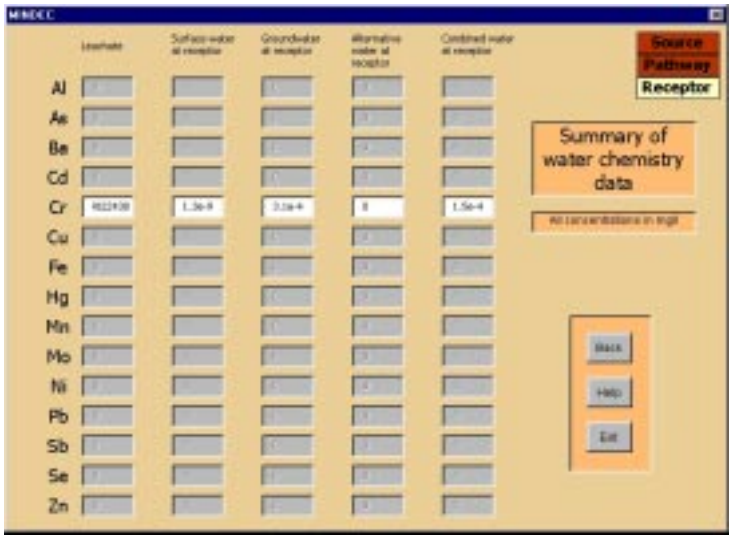
### **4.5.21** *Source Term* **M***odule*




Select an appropriate option button to either:

- Open a previously saved MINDEC scenario (*.mdc) file; or,
- Create a new scenario with leachate contaminant concentration data to be entered by the user; or,
- Create a new scenario with leachate contaminant concentration data to be estimated by MINDEC: or,
- Carry out a human health risk assessment using contaminant concentrations in water at the receptor site (i.e. with no consideration of source term or transport pathways).

### **4.5.22** *Summary of Water Chemistry* **D***ata*

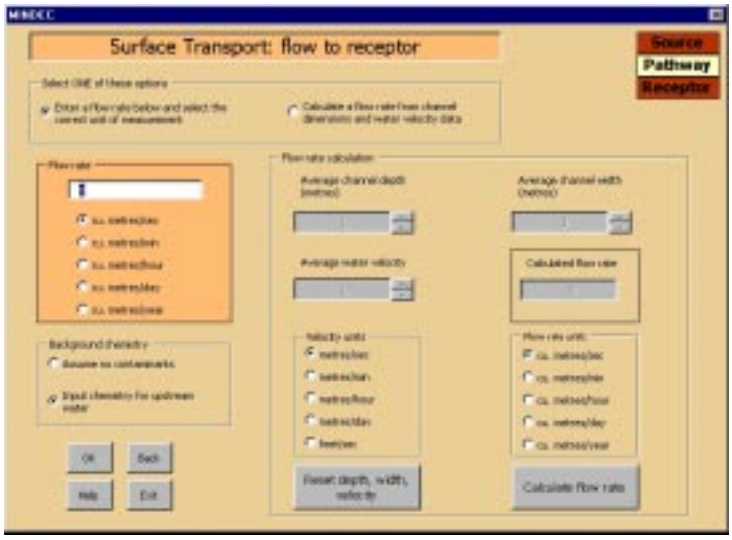



This screen presents a summary of calculated concentrations for waters from different sources at the receptor site together with leachate contaminant concentrations.

The 'Combined water at receptor' concentrations represent the average concentrations in water ingested by the consumer (receptor) taking into account the proportions of water from the different sources that are consumed. This set of concentration values is then used as the basis for the human health risk, assessment calculations.

These concentration results should be interpreted bearing in mind the large number of assumptions that are inherent within the modelling process. It is likely that they will not equate to actual concentrations at the receptor site but can be used as ‘best estimate’ values for the purposes of site prioritisation.

### **4.5.23** *Surface Transport: flow to receptor*




MINDEC requires a flow rate for the surface watercourse that transports leachate to the receptor (as measured upstream of the point at which the leachate enters the watercourse). This flow rate is used to calculate the extent of contaminant dilution within the watercourse.

Input options for the surface water flow rate are as follows:

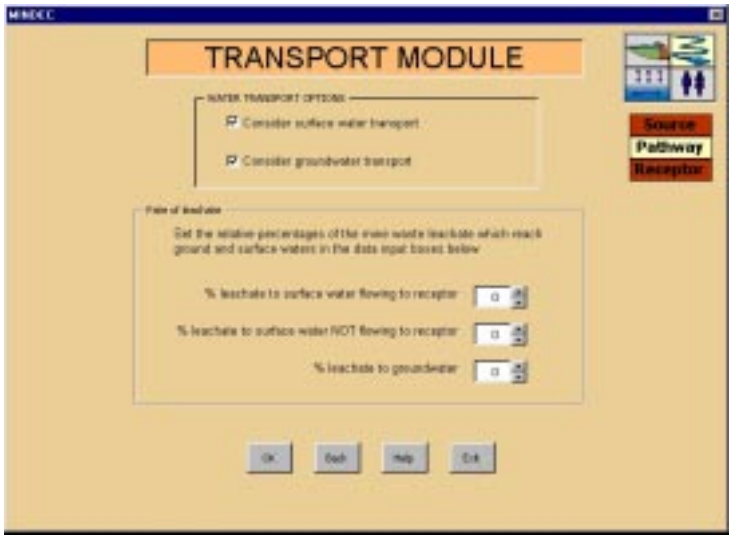
1. Enter a flow rate value directly (and select appropriate flow rate units); or,
2. enter channel dimensions (width and depth) and water velocity (and select appropriate velocity units). Then press the 'Calculate flow rate' button to calculate a flow rate. The 'Reset depth, width, velocity' button can be pressed if necessary to adjust the channel dimension and/or water velocity data. The calculated flow rate can be viewed in a number of different units by selecting the appropriate option button. Selecting a different unit will not affect the dilution calculations carried out by MINDEC.

Use the 'Background chemistry' option buttons to input contaminant concentrations for the surface water upstream from the leachate entry point or allow the program to assume that this water is uncontaminated.

The estimation of a surface water flow rate for the purposes of the dilution calculations should be carried out bearing in mind the need to include any additional tributary waterways which contribute water between the leachate source and the receptor.

Where Eh/pH conditions are suitable, precipitation and/or sorption (especially onto precipitated ochre deposits) may substantially reduce contaminant concentrations in surface waters. As these processes are difficult to quantify, MINDEC takes a conservative approach by only considering the effect of dilution in surface waters.

### 4.5.24 *Transport* **M***odule*




Use the option buttons to choose whether to consider surface and/or groundwater transport of leachate.

Then enter percentage values for the distribution of leachate between:

- surface water which flows to the receptor site;
- surface water which does not flow to the receptor site; and,
- groundwater.

These values will be difficult to establish for most sites and it may be necessary to run the model with a number of different estimates for these values. Some careful interpretation of transport pathways may be required in order to establish appropriate percentage values for these various sources, since some water may arrive at the receptor via a mixed surface/groundwater path. For example, water abstracted from a well immediately adjacent to a river might contain contaminants that have been transported largely within surface water before being drawn into the well. It would therefore be more appropriate for MINDEC to consider this water as surface water rather than groundwater since groundwater transport calculations would over-estimate travel times and mis-calculate the extent of any dilution and dispersion.
Similarly, careful consideration should be given to the possibility that contaminants might reach the receptor after migrating first through groundwater and then discharging into surface water.

Click on the navigation images in the top-right corner of the window to move directly backwards to the MINDEC source term or leachate flux screens if required. Note that it is not possible to jump forwards to the Receptor screen.

### **4.5.25** *Water **Q**uality Standards*

Select a water quality standard from the drop-down menu, with which to compare the leachate contaminant concentrations. The same set of standards will be used to compare the calculated concentrations at the receptor at a later stage in the program.
MINDEC is initially supplied with 3 sets of water quality standard data:

1. *World **H**ealth **O**rgani**z**ation* (WHO) drinking water guidelines (and concentrations likely to give rise to complaints from consumers)
2. ***E**uropean **U**nion* (EU) drinking water standards
3. ***U**nited **K**ingdom* (UK) drinking water standards

Additional water quality standards can be added, edited or deleted by the user by clicking on the 'Add/Edit' button. A data form will appear allowing existing data sets to be edited or deleted and new data sets to be added. The WHO, EU and UK data sets can also be updated in the same way if required. A 'Reset' button is also provided to allow the user to re-set the WHO, EU and UK standards to their default values if these have been edited in error. Pressing this button will not affect any user-defined data sets.

One of the water quality standard data sets can be selected as the default data set by clicking on the 'Set as default' check box. The selected standard data set will then appear as the default standard whenever MINDEC is run subsequently.

The water quality standards data are held in an Excel file called ***R**efdata.xls*. If MINDEC cannot find this file it may prompt the user to locate it. If the file is still not available then the WHO drinking water guidelines will be used as the default standard. No other data sets are available in this case.

As MINDEC finds the end of the database by looking for the first empty record in the data set title field it is important not to introduce blank records into the middle of the database. If these are introduced during editing, they must be removed by clicking on the 'Edit' button or by editing the Refdata.xls spreadsheet independently of MINDEC.

## 4.6 On-screen help

Help information is available using the Help buttons on the program screens. The Help Contents page provides a structured list of available topics, under the headings:

- How to use MINDEC help
- MINDEC: background
- MINDEC program screens

Click on a topic to view the appropriate page of information. For help with a particular program screen look for the appropriate screen title in the list under 'MINDEC program screens'.

The same help pages are also available from the Index that provides an alphabetical list of all available help topics.

A search facility is also available by clicking on 'Index' followed by 'Find'. Use Find to search for any word in the help pages text.

## 4.7 Troubleshooting and Technical support

For further information and technical support, contact the following e-mail address: mindec.enquiries@bgs.ac.uk.

# 5 *G*LO*SS*ARY

**A***bsorption*: the incorporation of a chemical into a solid or liquid.

**A***dsorption*: the incorporation of a chemical onto the surface of a solid or liquid.

**A***dvection*-**D***ispersion* **E***quation* (ADE): the differential equation that describes the transport of a contaminant in a porous medium aquifer. It is a statement of the law of conservation of mass. (Freeze and Cherry 1979) provide a derivation of this equation for the interested reader.

**A***quifer*: a geological unit that is sufficiently transmissive to yield significant quantities of water.

**A***quifer* P*roperties*: the range of physical variables particular to a rock unit that affect the movement of water and contaminants through that unit. Aquifer properties include hydraulic conductivity, porosity and dispersivity.

**A***ttenuation*: the reduction in contaminant concentration due to physical, chemical or biological processes as it passes through a medium.

**A***veraging Time*: in risk assessment calculations the length of time over which the dose is averaged. For carcinogenic risk it is the average life expectancy. For average daily dose calculations it is 365 days (i.e. one year).

*Buffering* P*otential*: the potential of a mineral on dissolution to control the pH of a water and thereby prevent the build-up of acidity.

*Calcite*: a carbonate mineral of calcium with the formula $CaCO_3$.

*Carcinogenic* **R***isk*: is the increased risk of getting cancer due to exposure to a carcinogen. It is usually expressed as a probability.

*Contaminant* **L***inear* **V***elocity*: also known as the advective velocity. It is derived by dividing the Darcy velocity by the effective porosity.

**D***ispersivity*: a characteristic property of a porous medium with dimension [L]; a measure of the tendency of a solute to disperse within groundwater moving through the medium.

**E***h*: the potential of a half-cell measured against a standard hydrogen half-cell. It is measured in the field using a portable electrode and gives an indication of the reduction-oxidation potential of water.

**E***xposure* **F***requency*: the number of days per year a receptor is exposed to a contaminant. Needed to calculate the average daily dose.

**E***xposure* **D***uration*: the number of years a receptor is exposed to a carcinogen. Needed to calculate the lifetime average daily dose.

**F***lux*: the rate of mass transport of a contaminant.

**F***racture* **F***low*: groundwater flow through fractures.

*Groundwater*: sub-surface water that occupies the saturated zone.

*Groundwater* **A***bstraction*: the withdrawal of groundwater as a water supply.

**H***alf-life*: the time taken for one half of a substance to decay.

**H***a***z***ard* **Q***uotient* **(HQ)**: the ratio between the average daily dose and the reference dose. An HQ>1 indicates the existence of a toxic risk.

**H***ead Gradient*: also known as the hydraulic gradient; the ratio between the difference in water level at two points divided by the distance between those two points, or the rate in change of head per unit distance of flow. It is a dimensionless quantity.

**H***ost* **R***ock*: a body of rock serving as a host for a mineral deposit.

**H***ydraulic Conductivity*: the constant of proportionality in Darcy's Law. The ratio between the flow of water through a rock and the hydraulic gradient across it.

*Ingestion* **R***ate*: for the purposes of MINDEC the ingestion rate is the contaminant concentration multiplied by the number of litres of contaminated water ingested. Units are mg/l/day.

**L***eachate*: the heavily mineralised solution formed by the percolation of rainfall and other surface waters through waste.

**L***ithology*: the physical description of a rock based on such characteristics as grain size and mineralogy.

**M***atrix* **F***low*: groundwater flow through the interconnected porosity of a rock matrix.

P*athway*: the route taken by contaminants from the source to the receptor. In MINDEC the pathways considered are surface water and groundwater.

P*ermeability*: the capacity of a porous rock to transmit water.

*p***H**: a measure of the activity of hydrogen ions in solution. In the field it is determined with an electrode; a pH<7 is acidic and a pH>7 is alkaline.

P*orosity*: the percentage of the volume of a rock or soil occupied by void space. The term 'effective porosity' refers to the percentage volume of interconnected void spaces through which flow can occur.

P*orous* **M***edium*: a lithology through which the principal flow mechanism is through connected pores.

P*rocess Water*: the water used on a mine for mineral processing.

P*yrite*: a sulphide mineral of iron. It is a common mineral in many ore deposits.

**R***eceptor*: living beings or resources that may be exposed to and affected by contamination.

**R***echarge* **R***ate*: the rate at which effective precipitation (rainfall) moves through the unsaturated zone to the water table.

**R***eference* **D***ose*: an estimate of the exposure to a toxic contaminant that can occur for a prolonged period without adverse health effects.

**R***etardation*: a measure of the reduction in solute velocity relative to the flowing groundwater due to processes such as adsorption.

**R***isk* **A***ssessment*: the process of estimating the risks of adverse health effects or environmental impacts due to exposure to a contaminant.

*Scenario*: a conceptual model of a site that considers a specific set of parameter inputs. Scenario analysis can be used to check model sensitivity to changes in a particular parameter.

*Slope* **F***actor*: a mathematical description of the dose of a contaminant received and the incidence of tumour development. The function is usually considered to be linear in the low dose range.

*Sorption*: a term including both adsorption and absorption.

*Source Term*: the quantity and concentration of a pollutant discharged at the pollution source.

*Sulphide* **O***xidation*: the natural process in which sulphide is converted to sulphate.

*Toxic* **R***isk*: the relationship between the average daily dose and the reference dose. In MINDEC the Hazard Quotient is used as a measure of toxic risk.

*Transport*: the movement of contaminants away from the source. The transport processes considered in MINDEC are surface water flow and groundwater flow.

**U***nsaturated* **Z***one*: the zone between the surface and the water table in which the water pressure is less than atmospheric i.e. the zone is in suction.

*Water* **Q***uality Standard* **(***W***Q***S***)**: a set of maximum allowable concentrations of contaminants in water.

*W***Q***S* **E***xceedance Index*: a numerical value used in MINDEC as a measure of the departure of water quality from the WQS.

# 6 R*eferences*

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